CLAIMS

We claim:

1. A computer implemented method to search a heterogenous compound database for molecules which are likely to have the same biological activity as a known query molecule comprising the following steps:

a) defining fragments of a query molecule and a database molecules according to a defined set of rules;

b) generating shape descriptors for the query molecule and database molecule fragments; and

c) using the shape descriptors, identifying the database molecule which has a shape similar to the query molecule.

2. A computer implemented method to search a heterogenous compound database for molecules which are likely to have the same biological activity as a known query molecule comprising the following steps:

a) fragmenting a query molecule according to a defined set of rules;

b) topomerically aligning the query molecule fragments to generate a topomeric conformation;

c) generating the interaction energies between a probe and the atoms in the topomerically aligned query fragments at all intersection points in a three dimensional grid surrounding the aligned query fragments;

d) fragmenting a database compound according to a defined set of rules;

e) topomerically aligning the database molecule fragments to generate a topomeric conformation;

f) generating the interaction energies between a probe and the atoms in the topomerically aligned database fragments at all intersection points in a three dimensional grid surrounding the aligned query fragments;

g) determining the similarity between query and database fragments by the root sum square differences in the field values; and

h) identify the molecule in the database most similar to the query molecule as that molecule having the smallest field value difference in its fragments.